Chapter 6: Linear Model Selection & Regularization

In the regression setting, the standard linear model is commonly used to describe the relationship between a response Y and a set of variables $X_1, \ldots, X_p$.

$$Y = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p + \epsilon$$

typically fit w/ least squares

Upcoming: more general models (non-linear)

The linear model has distinct advantages in terms of inference and is often surprisingly competitive for prediction. How can it be improved?

replace least squares w/ alternative fitting procedures.

We can yield both better *prediction accuracy* and *model interpretability*:

prediction accuracy: if true relationship is ≈ linear => least squares will have low bias.

If $n >> p$ => also have low variance => perform well on test data!

If n not much larger than p => high variability => poor performance.

If $p > n$ => no longer have a unique solution => variance = ∞ => cannot be used at all!

goal: reduce variance without adding too much bias.

model interpretability: often many variables used in a regression are not associated w/ response.

By removing (setting $\hat{\beta}_i = 0$), we can obtain a more easily interpretable model.

Note: least squares will hardly ever result in $\hat{\beta}_i = 0$.

=> need variable selection.

Same ideas apply to logistic regression.

1 Subset Selection

We consider methods for selecting subsets of predictors.

1.1 Best Subset Selection.

To perform *best subset selection*, we fit a separate least squares regression for each possible combination of the p predictors. $\binom{p}{2} = \frac{p(p-1)}{2}$ models with exactly 2 predictors, etc.

Algorithm:

1. Let $\mathcal{M}_0$ denote the model with no predictors.
2. For $k = 1, \ldots, p$
   (a) Fit all $\binom{p}{k}$ models that contain k predictors.
   (b) Pick the best of those (call it $\mathcal{M}_k$). "Best" is defined by $\downarrow$RSS ($\uparrow R^2$).
3. Select a single best model from $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using CV error, C_p, AIC/BIC, or adjusted R^2 (traditional metrics, more later.)

Why can't we use R^2 for step 3? as $p\uparrow$, $R^2\uparrow$ always. Why might we not want to do this at all? computation. Fitting 2^p models! $p = 10 \Rightarrow$ 1000 models.

We can perform something similar with logistic regression.

1.2 Stepwise Selection

For computational reasons, best subset selection cannot be performed for very large p. → "impossible" with $p \geq 40$.

Best subset may also subset when p large because w/ a large search space can find good models in training that perform poorly on test data
$\Rightarrow$ high variability & overfitting can occur.

Stepwise selection is a computationally efficient procedure that considers a much smaller subset of models.

Forward Stepwise Selection: start with no predictors and add one predictor at a time until all predictors are in the model, choose the "best" from these.

1. Let $\mathcal{M}_0$ denote the null model - no predictors
2. For $k = 0, \ldots, p-1$
   (a) Consider $p-k$ models that augment the predictors in $\mathcal{M}_k$ w/ 1 additional predictor.
   (b) Choose the best among these $p-k$ and call it $\mathcal{M}_{k+1}$ ($\uparrow R^2$).
3. Select a single best model from $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using CV error, C_p, AIC/BIC, or adjusted R^2.

Now we fit $1 + \sum_{k=0}^{p-1}(p-k) = 1 + \frac{p(p+1)}{2}$ models!

Backward Stepwise Selection: Begin w/ full model and take predictors away one at a time until you get to the null model.

1. Let $\mathcal{M}_p$ denote the full model, contains all predictors.
2. For $k = p, p-1, \ldots, 1$:
   (a) consider all models (k) that contain all but one of the predictors in $\mathcal{M}_k$ ($k-1$ predictors).
   (b) Choose the best among them, call it $\mathcal{M}_{k-1}$ ($\uparrow R^2$).
3. Select the single best model from $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using CV, C_p, AIC/BIC, or adjusted R^2.

* Neither forward nor backwards stepwise selection are guaranteed to find the best model containing a subset of the p predictors.

Forward Selection can be used when $p > n$ (but only up to $n-1$ predictors (not up to p)).

1.3 Choosing the Optimal Model

Best subset, forward selection, backward selection all need a way to pick the "best" model – according to test error.

- RSS & R^2 are proxy for training error $\Rightarrow$ not estimates of test error
  - ↳ (1) estimate this directly (CV) or
  - (2) adjust training errors for model size.

(2) $C_p = \frac{1}{n}\left(\text{RSS} + 2d\hat{\sigma}^2\right)$ — $\hat{\sigma}^2$: estimate of variance of ε (full model).

RSS: subset model. d: # predictors in subset model.

adds a penalty to training error (RSS) to adjust for underestimation of test error.

(choose model w/ lowest value).

(2) AIC & BIC can get for models fit w/ MLE

$$\text{AIC} = \frac{1}{n\hat{\sigma}^2}\left(\text{RSS} + 2d\hat{\sigma}^2\right).$$

$$\text{BIC} = \frac{1}{n\hat{\sigma}^2}\left(\text{RSS} + \log(n)\, d\hat{\sigma}^2\right).$$

choose model w/ lowest AIC or BIC.

↑ $\log(n) > 2$ for $n > 7$ $\Rightarrow$ heavier penalty on models w/ many variables $\Rightarrow$ results in smaller models.

(2) Adjusted R^2 (only for least squares).

$$R^2 = 1 - \frac{\text{RSS}}{\text{TSS}}$$ Always ↑ as d ↑

$$\text{Adj } R^2 = 1 - \frac{\text{RSS}/(n-d-1)}{\text{TSS}/(n-1)}$$ choose model w/ highest Adj R^2.

(1) Validation and Cross-Validation

Directly estimate test error w/ Validation or CV and choose model w/ lowest estimated error.

Very general (can be used for any model) even when it's not clear how many "predictors" we have.

Now have fast computers $\Rightarrow$ these are preferred.

2 Shrinkage Methods

The subset selection methods involve using least squares to fit a linear model that contains a subset of the predictors. As an alternative, we can fit a model with all p predictors using a technique that constrains (*regularizes*) the estimates.

↳ shrinks estimates towards zero.

Shrinking the coefficient estimates can significantly reduce their variance!

Help us to avoid overfitting!

2.1 Ridge Regression

Recall that the least squares fitting procedure estimates $\beta_1, \ldots, \beta_p$ using values that minimize

$$RSS = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij}\right)^2$$

residual sum of squares.

$\hat{\beta}^R$

Ridge Regression is similar to least squares, except that the coefficients are estimated by minimizing

$$\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij}\right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 = RSS + \lambda \sum_{j=1}^{p} \beta_j^2$$

note we are not penalizing β_0
we want to penalize the relationships, not the intercept
(mean value of response when $x_{i1} = \cdots = x_{ip} = 0$).

$\lambda \geq 0$ tuning parameter (determine separately from fitting).

trades off 2 criteria: minimize RSS to fit data well

minimize $\lambda \sum_{j=1}^{p} \beta_j^2$ "shrinkage penalty" will be small when β_j close to zero $\Rightarrow$ shrink estimates towards zero.

The tuning parameter λ serves to control the impact on the regression parameters.

When $\lambda = 0$, penalty has no effect $\Rightarrow$ ridge regression = least squares.

As $\lambda \to \infty$, impact of penalty grows $\Rightarrow$ $\hat{\beta}^R \to 0$.

Ridge regression will produce a different set of coefficients for each penalty ($\hat{\beta}^R_\lambda$).

Selecting a good λ is critical! How to choose? Cross validation!

The standard least squares coefficient estimates are scale invariant.

In contrast, the ridge regression coefficients $\hat{\beta}_\lambda^R$ can change substantially when multiplying a given predictor by a constant.

Therefore, it is best to apply ridge regression *after standardizing the predictors* so that they are on the same scale:

Why does ridge regression work?

2.2 The Lasso

Ridge regression does have one obvious disadvantage.

This may not be a problem for prediction accuracy, but it could be a challenge for model interpretation when p is very large.

The *lasso* is an alternative that overcomes this disadvantage. The lasso coefficients $\hat{\beta}_\lambda^L$ minimize

As with ridge regression, the lasso shrinks the coefficient estimates towards zero.

As a result, lasso models are generally easier to interpret.

Why does the lasso result in estimates that are exactly equal to zero but ridge regression does not? One can show that the lasso and ridge regression coefficient estimates solve the following problems

In other words, when we perform the lasso we are trying to find the set of coefficient estimates that lead to the smalled RSS, subject to the contraint that there is a budget s for how large $\sum_{j=1}^{p} |\beta_j|$ can be.

2.3 Tuning

We still need a mechanism by which we can determine which of the models under consideration is “best”.

For both the lasso and ridge regression, we need to select λ (or the budget s).

How?

3 Dimension Reduction Methods

So far we have controlled variance in two ways:

We now explore a class of approaches that

We refer to these techniques as *dimension reduction* methods.

The term *dimension reduction* comes from the fact that this approach reduces the problem of estimating $p + 1$ coefficients to the problem of estimating $M + 1$ coefficients where $M < p$.

Dimension reduction serves to constrain β_j, since now they must take a particular form.

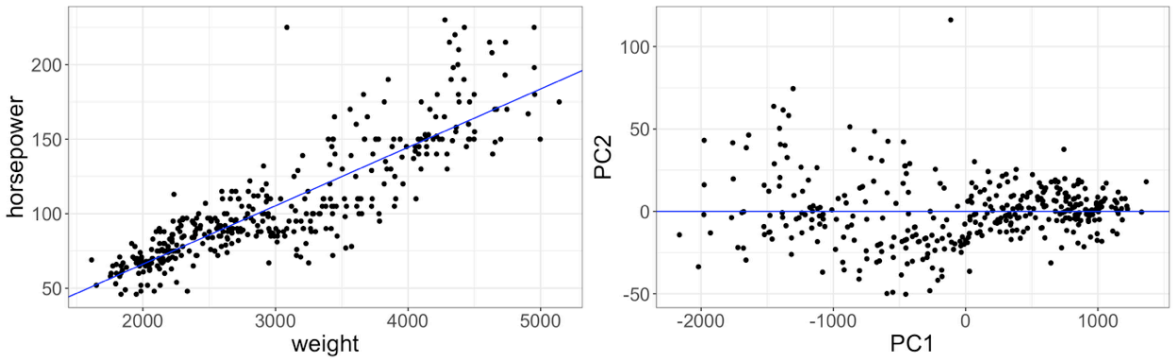
All dimension reduction methods work in two steps.

3.1 Principle Component Regression

Principal Components Analysis (PCA) is a popular approach for deriving a low-dimensional set of features from a large set of variables.

The *first principal component* directions of the data is that along which the obervations vary the most.

We can construct up to p principal components, where the 2nd principal component is a linear combination of the variables that are uncorrelated to the first principal component and has the largest variance subject to this constraint.



The Principal Components Regression approach (PCR) involves

1.

2.

Key idea:

In other words, we assume that the directions in which $X_1, \ldots, X_p$ show the most variation are the directions that are associated with Y.

How to choose M, the number of components?

Note: PCR is not feature selection!

3.2 Partial Least Squares

The PCR approach involved identifying linear combinations that best represent the predictors $X_1, \ldots, X_p$.

Consequently, PCR suffers from a drawback

Alternatively, *partial least squares (PLS)* is a supervised version.

Roughly speaking, the PLS approach attempts to find directions that help explain both the reponse and the predictors.

The first PLS direction is computed,

To identify the second PLS direction,

As with PCR, the number of partial least squares directions is chosen as a tuning parameter.

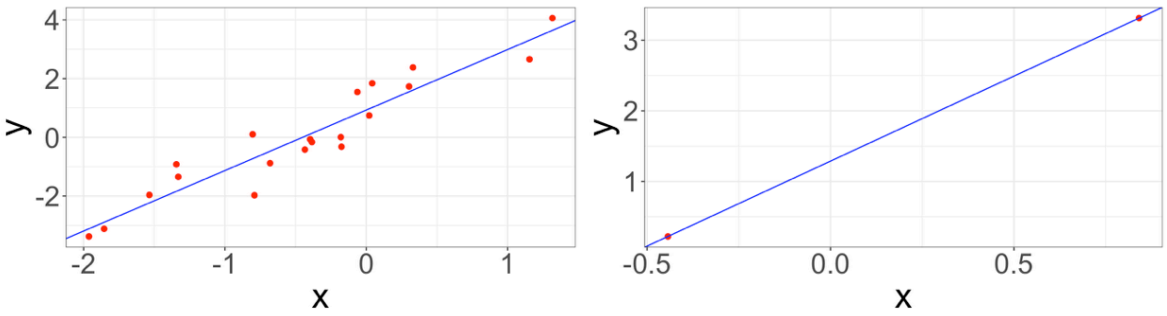
4 Considerations in High Dimensions

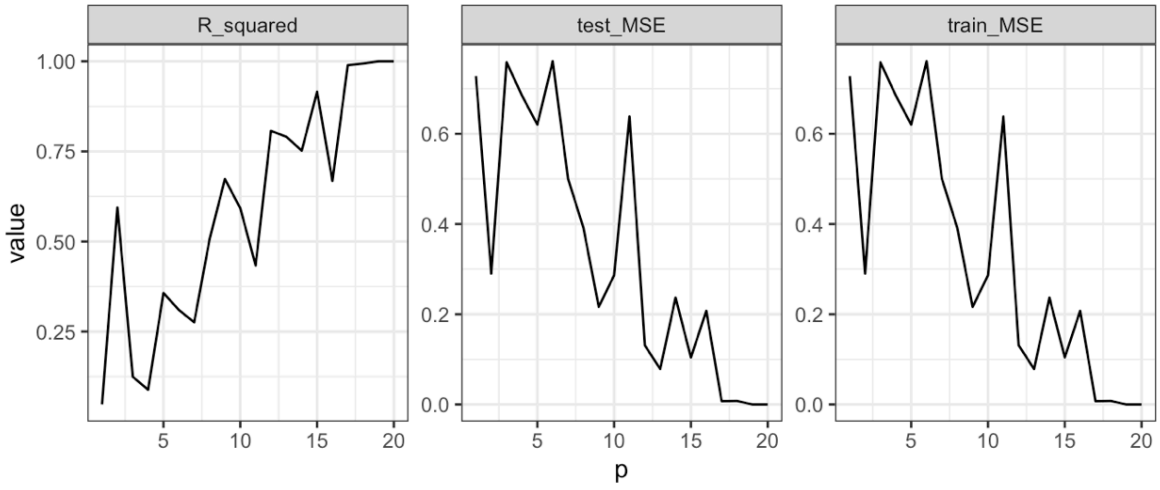
Most traditional statistical techniques for regression and classification are intendend for the low-dimensional setting.

In the past 25 years, new technologies have changed the way that data are collected in many fields. It is not commonplace to collect an almost unlimited number of feature measurements.

Data sets containing more features than observations are often referred to as *high-dimensional*.

What can go wrong in high dimensions?





Many of the methods that we've seen for fitting *less flexible* models work well in the high-dimension setting.

1.

2.

3.

When we perform the lasso, ridge regression, or other regression procedures in the high-dimensional setting, we must be careful how we report our results.